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Determination of the Order Parameter of the CuPt-ordered Semiconductor Ternary Alloys by X-ray Diffraction

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Beamline(s): X14A

Introduction: The order parameter of an atomically ordered semiconductor alloy is essential for understanding the electronic and optoelectronic behavior of the alloy. Here, we present an x-ray method for the quantitative determination of the order parameter of atomically ordered semiconductor alloy films.

Methods and Materials: As an example, we studied several CuPt-ordered $GaInP_2$ alloy films grown on a GaAs (001) substrate with either single or double ordering variants. We used a skew diffraction geometry which permits access to Bragg diffraction that is not possible in a conventional co-planar geometry. Radial (hhh) scans were used to avoid possible effects from defects such as micro-twins and stacking faults.[1]

Results: The structure factor of an atomically ordered alloy crystal can be expressed in terms of contributions from a random structure, atomic ordering, and statistic atomic displacements.[2] This last term causes an additional modulation to the intensity profile, therefore can be used to measure the order parameter. In Fig. 1, the calculated intensities of the ordering peaks with and without considering the atomic displacements were shown for a $GaInP_2$ sample with an order parameter of 0.5. It is clear that atomic displacements are able to cause observable changes in the intensities of the ordering peaks. Such changes have indeed been observed in previous measurements of several differently ordered alloys[3,4] and in this experiment. Fig. 2 shows the measured (-3/2,3/2,3/2) and (-5/2,5/2,5/2) peaks for one of our samples. The (-5/2,5/2,5/2) peak is obviously stronger than the (-3/2,3/2,3/2) one, and this is not expected from simple considerations of atomic form factor and atomic ordering and Debye-Waller factors. We introduced theoretically calculated atomic displacements into our calculations and compared the measured and calculated relative intensities of two ordering peaks (-3/2,3/2,3/2) and (-5/2,5/2,5/2). In this way, we obtained the order parameters of several CuPt-order $GaInP_2$ alloy films.

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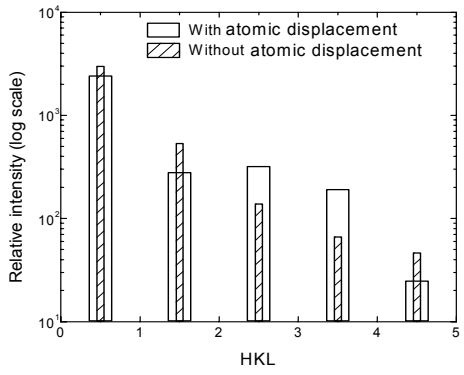

Fig. 1 Calculated intensities of an ordered GaInP alloy, with and without considering atomic displacements.

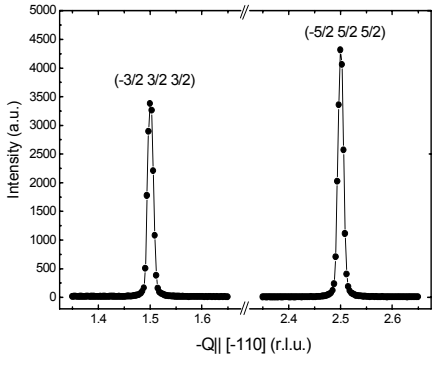

Fig. 2 Experimental (-3/2,3/2,3/2) and (-5/2,5/2,5/2) ordering peaks.